Progress on a Full Radius Electromagnetic Gyrokinetic Code

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Abstract. We describe work in progress to formulate a general geometry full radius nonlinear electromagnetic gyrokinetic code to simulate high-n turbulence and transport in tokamaks. The code employs continuum (fluid-like) methods in a 5-dimensional grid space. The code has three modes of operation: (1) flux tube with periodic radial boundary condition (i.e., a high-n ballooning mode representation with $\Delta n \approx 10$); (2) a full radius wedge code ($\Delta n \approx 10$) to study profiles shear effects; and (3) a full torus ($\Delta n = 1$) code to study coupling to low-n MHD.

Introduction and Motivation

The electromagnetic gyrokinetic equations encompass the full physics of turbulence and transport due to low-frequency motion (less than the cyclotron frequency) for systems where the ion gyroradius is small compared to the variation length of the magnetic field. Heretofore, such linear [1] and nonlinear equations [2] have been formulated in the high-n ballooning mode representation (BMR) in which the relative ion gyroradius, $\rho_* = \rho_i/a$, vanishes. Previous simulations have been largely limited to adiabatic electrons, electrostatic perturbations, and use particle (Monte-Carlo) methods which treat only ion temperature gradient mode (ITG) turbulence in infinite aspect ratio circular s-α model geometry. Related work [3] is in progress on a nonlinear ballooning-space code employing successful implicit techniques [4] to treat fast passing electrons and electromagnetic dynamics. The BMR uses a radial Fourier transform or flux tube with radially periodic boundary conditions. The present work avoids this transform and stays in the physical (r,θ) space so as to treat the effects of slow radial equilibrium profile variations on the turbulence. It is now well known from gyrofluid ballooning mode simulations of ITG turbulence that profile shear in the equilibrium E×B velocity can completely stabilize the turbulence when the shear rate, $\gamma_E = (r/q)\partial_r(qV_{ExB}/r)$, is comparable to the maximum linear ballooning mode rate [5]. However in reality the shear rate in the diamagnetic velocity is comparable with that in the E×B velocity and is expected to have a similar effect. This and other profile variations can only be treated with a full radius code which retains finite ρ_*. In addition the code should provide a more physical measure of non-local avalanche and “action at a distance” [6] effects. A final and more distant motivation is to study the interaction of high-n micro-scale turbulence with low-n global MHD modes. The code uses Miller's local equilibrium [7] which generalizes the s-α model by retaining arbitrary aspect ratio, Shafranov shift, ellipticity, and triangularity. Thus we expect to have a good description of low-n MHD modes when running the code as a full torus with toroidal mode numbers n = 0,1,2,…100, rather than a full radius wedge (1/10th torus) with n = 0,10,20,…100.

Coordinate System

We designate a coordinate system (r,θ,α) where r is the midplane minor radius used as a flux-surface label, and θ is a poloidal angle associated with Miller's local equilibrium [7]. We use the field aligned variable $\alpha = \zeta - \int_0^\theta \hat{q} d\theta$ in place of the toroidal angle, ζ, where $\hat{q} = \hat{b}\cdot\nabla\zeta / \hat{b}\cdot\nabla\theta$ is the local safety factor. Accordingly, $\hat{b}\cdot\nabla\alpha = 0$ and $\hat{b}\cdot\nabla r = 0$. Perturbations are Fourier decomposed as $\phi = \Sigma_n \phi_n(r,\theta)\exp(-in\alpha)$. To ensure periodicity in the physical field ϕ, we require $\phi_n(r,\pi) = \phi_n(r,-\pi)\exp(-in2\pi q)$ where $q = \int_0^{2\pi} \hat{q} d\theta / 2\pi$ is the flux surface average of $\hat{q}$. If q(r) = m/n for any m we say r is a singular surface, in which case the periodicity *phase factor*, $\exp(-in2\pi q)$, is unity. The parallel field derivative is $\nabla_\parallel = (\hat{b}\cdot\nabla\theta)\partial_\theta$. We designate a local orthogonal triad $[\hat{x},\hat{y},\hat{b}]$ at (r,θ) where $\hat{y} = \hat{x}\times\hat{b}$.

The perpendicular derivatives acting on the *fast* $\exp(-in\alpha)$ part are given by $\nabla^f_{\perp y} = -in\nabla\alpha \cdot \hat{b} \times \hat{x} = ik_\theta \eta_q(\theta)$ where $k_\theta \equiv nq/r$ and $\eta_q(\theta) = (rB/RB_\theta)/q$, and $\nabla^f_{\perp x} = -in\nabla\alpha \cdot \hat{x} = ik_\theta \eta_q(\theta)\eta_k(\theta)$. In the BMR only the *fast* part of the in-flux-surface perpendicular derivative (y-part) is considered. We have an additional *slow* derivative on $\phi_n(r,\theta)$; namely $\nabla^S_{\perp y} = (B_t/B_p)(\hat{b} \cdot \nabla\theta)\partial_\theta$. In general the r-derivative on $\phi_n(r,\theta)$ is assumed to be a mixture of *fast* and *slow* with $\nabla^{fs} = |\nabla r|\partial_r$. In the circular $\hat{s} - \alpha$ model we have the reductions $(\hat{b} \cdot \nabla\theta) \Rightarrow 1/R_0 q$, $\eta_q(\theta) \Rightarrow 1$, $\eta_k(\theta) \Rightarrow \hat{s}\theta - \alpha\sin\theta$, and $|\nabla r| \Rightarrow 1$ [7]. To do the gyroaverage we write $\langle\phi\rangle = \Sigma_n \exp(-in\alpha)\langle\phi\rangle_n$ and expand the arguments of $\langle\phi\rangle_n$ to first order in $\rho_\perp/r$, so that $\langle\phi\rangle_n = \oint d\alpha_g/2\pi \exp(-in\bar{\rho}_\perp \cdot \nabla\alpha)\phi_n(r + \bar{\rho}_\perp \cdot \nabla r, \theta + \bar{\rho}_\perp \cdot \nabla\theta)$. As a first approximation the *slow* $\bar{\rho}_\perp \cdot \nabla\theta$ can be neglected.

Normalization

We choose $T_e(0)$ and $n_e(0)$ as the units of temperature and density. The unit of length is the midplane radius of the last closed flux surface, a. The unit of velocity is $c_{s0} = [T_e(0)/M_i]^{1/2}$, and the unit of time is a/c_{s0}. The normalized potentials are $|e|\phi/T_e(0) = \hat{\phi}$ and $(c_{s0}/c)|e|A/T_{e0} = \hat{A}$. We normalize the non-adiabatic component of the distribution function by $g = \hat{g}(r,\theta,\hat{\varepsilon},\lambda,\sigma)n_e(0)F_M$, where $\hat{\varepsilon} = \varepsilon/T$ is the normalized energy, $\lambda = \mu/\varepsilon$ is the pitch angle, $\sigma = \mathrm{sgn}(v_\|)$, and F_M is the background Maxwellian. Since ε and λ are constants of motion in the gyrokinetic equation, the radial derivative of g is $\partial_r\hat{g} = n_e(0)F_M D_r\hat{g}$ where $D_r\hat{g} = \partial_r\hat{g} + (\hat{\varepsilon}/L_T)\partial_{\hat{\varepsilon}}\hat{g} - ((\hat{\varepsilon} - 3/2)/L_T)\hat{g}$ and $1/L_T$ is the logarithmic temperature gradient. The latter terms in $D_r\hat{g}$ are absent in the BMR with vanishing $\rho*$. The normalization introduces three parameters: the central ρ^* [$\rho_{s0} = c_{s0}/(eB_0/M_i c)$], Debye length λ_{D0}, and electron beta β_{e0}.

Gyrokinetic Equations

In normalized units, denoting a gyroaverage by $\langle\ \rangle$, Poisson and Ampère's equations are

$$-\lambda_{D0}^2 \nabla^2 \hat{\phi} = \sum_s \iint z\left[-z\hat{n}/\hat{T}\hat{\phi} + \langle g\rangle\right], \quad \text{and} \quad -\rho_{s0}^2 \nabla^2 \hat{A}_\| = (\beta_{e0}/2)\sum_s \iint z\hat{v}_\| \langle\hat{g}\rangle ,$$

where the phase space integral $\iint \Rightarrow \Sigma_\sigma \pi^{-3/2} \int_0^\infty d\hat{\varepsilon}\hat{\varepsilon}^{1/2} \exp(-\hat{\varepsilon})(\pi/2)\int_0^{1/B} d\lambda B/(1-\lambda B)$.

Finally following Ref. [2], we can write the gyrokinetic equation as

$$\partial_i\hat{g} + v_\|(\hat{b} \cdot \hat{\nabla}\theta)\partial_\theta\hat{g}$$
$$= M\partial_i\langle\hat{U}\rangle - i\omega_E\left(-M\langle\hat{U}\rangle + \langle g\rangle\right) + i\varpi_D\hat{g} - i\hat{n}\varpi_* + \left\{\langle\hat{U}\rangle,\langle g\rangle\right\} - \left\{\langle g\rangle,\langle\hat{U}\rangle\right\} + C\hat{g} ,$$

where "hat" quantities are normalized, $M \equiv z\hat{n}/\hat{T}$ and $U = \hat{\phi} - \hat{v}_\|\hat{A}_\|$ is the effective potential. The low-n MHD approximation of neglecting $A_\perp$ while forcing the cuvature drift to equal the grad-B drift is very good even for high-n. The curvature drift operator which acts only on $\hat{g}$ is $\hat{\varpi}_D = -iz\hat{T}(2/R_0)\rho_{s0}(B_0/B)\{C(\theta,\hat{\varepsilon},\lambda)\ [inq/\hat{r}]\ + S(\theta,\varepsilon,\lambda)\ [i(nq/\hat{r})\eta_k + (|\nabla r|/\eta_q)D_{\hat{r}}]\}$ where C is the cosine-like normal curvature, S the sine-like geodesic curvature, and we define $[inq/\hat{r}] \equiv inq/\hat{r} + (B_t/B)(\hat{R}q/\hat{r})(\hat{b} \cdot \hat{\nabla}\theta)\partial_\theta$. [7]. Thus the diamagnetic term is $\varpi_* = -i(B_0/B_{unit})\rho_{s0}[inq/\hat{r}][1/\hat{L}_n + 1/\hat{L}_T(\hat{\varepsilon} - 3/2)]$ and $\hat{\omega}_E = -i(B_0/B_{unit})\partial_{\hat{r}}\hat{\Phi}_0\rho_{s0}[inq/\hat{r}]$ is the E×B equilibrium rotation frequency The nq/r terms are *fast* and the ∂_θ terms are *slow*.

$$\{X,Y\} \equiv \sum_{n',n''=n-n'} (B_0/B_{unit})\rho_{s0}[in''q/\hat{r}]X_{n''}\left[\partial_r + i(n'q/\hat{r})\eta_k\eta_q/|\nabla r|\right]Y_{n'} ,$$

where again we use D_r when ∂_r acts on g. C is the pitch angle scattering operator.

Numerical Method

Because the parallel electron term, $Lg = v_{\parallel}(\hat{b}\cdot\nabla\theta)\partial_\theta g$, is so fast, implicit methods must be used to advance U at the same time as the distribution g. Dropping the hat notation, the gyrokinetic equation can be differenced in a time-centered fashion $[1/\Delta t + \delta L]g(t+\Delta t) = (M/\Delta t)\langle U\rangle(t+\Delta t)H(t) = S_g$ where information at time t is given by $H = [1/\Delta t - (1-\delta)L]g(t) - (M/\Delta t)\langle U\rangle(t) + E(t)$, and E corresponds to the second line of the gyrokinetic equation. Note that $\delta = 1$ corresponds to fully implicit. The Green's function $G = (1/\Delta t + \delta L)^{-1}$ is discretized using 2-point θ-derivatives centered at j + 1/2. G is diagonal in the radial grid, and must account for trapped particle bouncing, and the *phase factor* on passing particles. Thus $g(t+\Delta t)_j = \Sigma_j G_{jj'}[(M/\Delta t)\langle U\rangle(t+\Delta t)_{j'+1/2} + \{\{g(t)\}\}_j$ where we have defined $\{\{g(t)\}\}_j = \Sigma_{j'} G_{jj'} H(t)_{j'+1/2}$ Defining $S_{\phi j}(t) = \Sigma_s \iint z^s \langle\{\{g^s(t)\}\}\rangle_j$ the Poisson equation becomes

$$-\lambda_{s0}^2\nabla^2\phi_j(t+\Delta t) - \Sigma_s z^s\{-M^2\phi_j(t+\Delta t) + \iint \langle\Sigma_{j'} G^s_{jj'}[(M^2/\Delta t)\ \langle U(t+\Delta t)\rangle]_{j'+1/2}\rangle\} = S_{\phi j}$$

With a similar equation for Ampère's law, we write an implicit field equation $\overline{M}\vec{V}(t+\Delta t) = \vec{S}(t)$ for $\vec{V} = \{\phi, A_{\parallel}\}$. Since the gyroaveraging essentially spans all radii m, $M_{jj'mm'}$ is a full matrix which must be inverted to get the response matrix R. R and G are computed once and stored. We expect to parallelize by assigning one radial grid to a processor. For $N_\theta = 32$, $N_r = 100$, $N_\varepsilon = 5$, $N_\lambda = 50$, $N_{fields} = 3$, $N_{species} = 2$, and $N_n = 10$, we find 14 MW×N_r is required to store the gyroaverage operator, 10 MW×N_r for R, 5MW×N_r for G. U and g storage is small and in total we should require less than 32 MW per processor (MW = megaword).

Reduction to Ballooning Mode Space and First Results

An important first step is to recover the BMR using the periodic boundary condition $\phi_n(\theta, r_s + \Delta r/2) = \phi_n(\theta, r_s - \Delta r/2)$ the limit $n_{max} \gg 1$ and $\rho_{s0} \ll 1$ such that $\rho_{s0}(n_{max}q/r)$ remains fixed near 1. All of the *slow* terms will become negligible compared to the *fast* terms. The BMR is a Fourier transform $\phi_n(\theta, r_s + x) = \Sigma_{k_x}\overline{\phi}_{n,k_x}(\theta)\exp(ik_x x)$ on an extended angle $-\infty<\theta<\infty$. We can rewrite the Fourier label as $k_x = \hat{s}k_\theta(\theta_0 + 2\pi p)$ where $k_\theta = nq(r_s)/r_s$, p is the "image index" which runs over all integers, and $\theta_0 \in [-\pi, \pi)$ is the discretized "ballooning angle label." Periodicity is preserved by requiring that the BMR space functions $\overline{\phi}_{n\theta_0 p}(\theta - 2p\pi) = \overline{\phi}_{n\theta_0 0}(\theta)\exp[inq(r_s)2\pi px]$. This property in ballooning space is entirely equivalent to the *phase factor* in real space (r,θ). We must assume that the ballooning modes are localized in θ, for example -3π to 3π. That means only first images p = ±1 need be retained. If we place the highest $J_* - 1$ image retained at half the Nyquist wave number (4 radial grids per wavelength), then we require a radial grid spacing $\delta r/\rho_{s0} < 1/[2J_*\hat{s}(k_\theta^{max}\rho_{s0})] = (\Delta_s/\rho_{s0})/(2J^*)$ where Δ_s is the space between singular surfaces. Note that $N_r = 2l_* J_*$ where $l_*(\theta_0/2\pi) = 0,1,.2...(l_* - 1)$. For nonlinear runs we expect $l_* = 20$ and $J_* = 2$ to suffice or a box of $80/(2\hat{s})$ gyrolengths ρ_{s0} which can either be concentrated over a distance with no significant profile variation or eventually over the full radius. To make a first linear illustration with $l_* = 1$ and $J_* = 2$, consider an adiabatic electron, electrostatic, $\hat{s} - \alpha$ circular case with, $\hat{s}$ = 0.25, α = 0, q = 2, $1/L_T = 6$, $1/L_n = 1$, $T_i/T_e = 1$, r = 1/2, and R = 1/3. Using $N_r = 4$ and N_θ = 32 on $\theta \in [-\pi, \pi)$ we have obtained the preliminary result (ω,γ) = (–0.257,0.312) (see Fig. 1) compared to Kotschenreuther's [4] code (–0.249,0.303) obtained on a $\theta \in [-3\pi, 3\pi]$ ballooning angle space. Thus we are using 2-dimensions to solve a normally 1-dimensional problem for the BMR. The added dimension will later allow us to treat the profile effects. Crucial to obtaining this result was the use of a spectral technique to evaluate radial derivatives and gyroaverages. For example the "harmonic derivative" is defined such that for any of the N_r allowed k_x's of the simulation box, $[\partial_r]_H \exp(ik_x x) = (ik_x)\exp(ik_x x)$. This results in radial derivative and gyroaveraging operators which connect all N_r gridpoints.

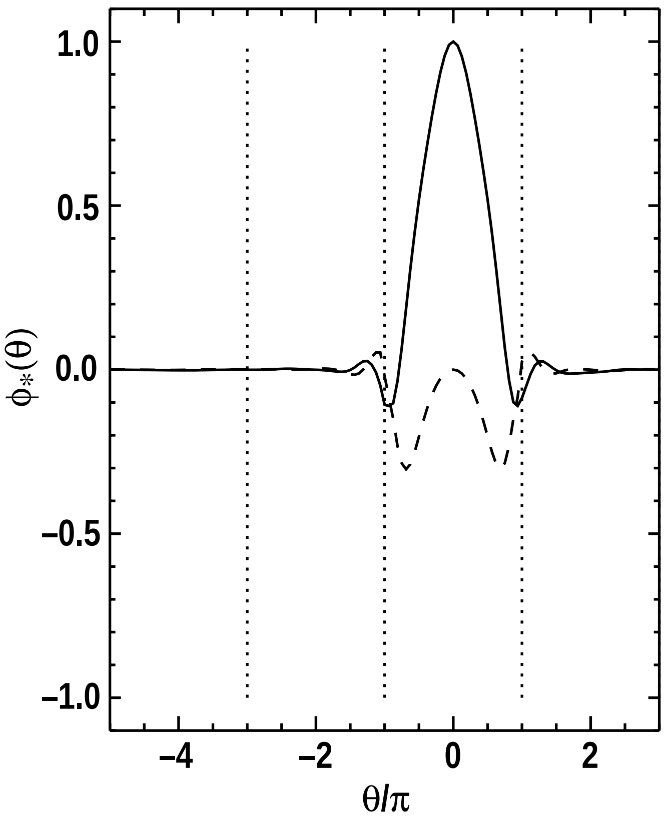

Fig. 1. Reconstruction of the example θ_0 = 0 ballooning mode using data from the real (r,θ) space full radius code. The latter was operated in flux tube mode with radially periodic boundary conditions. The [–5π,–3π) section is from the p = –2 component, [–3π, –π) from p = –1, [–π,π) from p = 0, and [π,3π) from p = 1. The real /imaginary part of the ϕ_* solution is shown as a solid/dashed curve.
$\phi_*(\theta + 2\pi p) = \bar{\phi}_{k_x}(\theta)$
where $k_x = \hat{s} k_\theta (2\pi p)$

The electrons pose a significant problem in r-space since the Landau damping layer $\Delta_e / \rho_{s0} = (Rq/\hat{s})(\omega/\omega_*)(m_e/2M_i)^{1/2}$ is impractical to resolve without a 100-fold increase in J_*. If any grid is within a distance Δ_e of a singular surface, it will over-weight the $k_{||} = 0$ passing electron dynamics (see Ref. [5] for discussion of this problem). The BMR avoids this by forcing 0 boundary conditions at the extended angle θ = ±3π (in our example) which properly nullifies $k_{||} = 0$ contribution, since its true weight is only $\Delta_e / \delta r$ and thus should be neglected. The preliminary version of our full radius code treats the $D_r g$ radial derivatives explicitly and eliminates the $k_{||} = 0$ contribution by an explicit inverse transform of the BMR 0 boundary conditions to r-space. This method works but we believe an implicit operator splitting method incorporating these operations will be more robust.

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